

RESULT 5

BXA2_CLOBO

Title: US-10-527-411-50

Perfect score: 5864

Sequence: 1 MEFVNKQFNYKDPVNGVDIA.....AAETHDVYSWSFHASLPETN
1127

ID BXA2_CLOBO STANDARD; PRT; 1295 AA.

AC Q45894; P77780;

DT 23-JAN-2002, integrated into UniProtKB/Swiss-Prot.

DT 23-JAN-2002, sequence version 2.

DT 11-JUL-2006, entry version 57.

DE Botulinum neurotoxin type A precursor (EC 3.4.24.69) (BoNT/A)

DE (Bontoxilysin-A) (BOTOX) [Contains: Botulinum neurotoxin A light-

DE chain; Botulinum neurotoxin A heavy-chain].

GN Name=botA; Synonyms=atx, bna;

OS Clostridium botulinum.

OC Bacteria; Firmicutes; Clostridia; Clostridiales; Clostridiaceae;

OC Clostridium.

OX NCBI_TaxID=1491;

RN [1]

RP NUCLEOTIDE SEQUENCE [GENOMIC DNA].

RC STRAIN=Type A / Kyoto-F;

RX MEDLINE=94143603; PubMed=8310180; DOI=10.1016/0923-2508(93)90004-L;

RA Willems A., East A.K., Lawson P.A., Collins M.D.;

RT "Sequence of the gene coding for the neurotoxin of Clostridium

RT botulinum type A associated with infant botulism: comparison with

RT other clostridial neurotoxins.";

RL Res. Microbiol. 144:547-556(1993).

RN [2]

RP NUCLEOTIDE SEQUENCE [GENOMIC DNA] OF 1-65.

RC STRAIN=Type A / Kyoto-F;

RX MEDLINE=97016817; PubMed=8863443;

RA East A.K., Bhandari M., Stacey J.M., Campbell K.D., Collins M.D.;

RT "Organization and phylogenetic interrelationships of genes encoding

RT components of the botulinum toxin complex in proteolytic Clostridium

RT botulinum types A, B, and F: evidence of chimeric sequences in the

RT gene encoding the nontoxic nonhemagglutinin component.";

RL Int. J. Syst. Bacteriol. 46:1105-1112(1996).

CC -!- FUNCTION: Inhibits acetylcholine release. The botulinum toxin

CC binds with high affinity to peripheral neuronal presynaptic

CC membrane to the secretory vesicle protein SV2. It binds directly

CC to the largest luminal loop of the three isoforms SV2A, SV2B and

CC SV2C. It is then internalized by receptor-mediated endocytosis.

CC The C-terminus of the heavy chain (H) is responsible for the

CC adherence of the toxin to the cell surface while the N-terminus

CC mediates transport of the light chain from the endocytic vesicle

CC to the cytosol. After translocation, the light chain (L)
 CC hydrolyzes the 197-Gln-|-Arg-198 bond in SNAP-25, thereby blocking
 CC neurotransmitter release. Inhibition of acetylcholine release
 CC results in flaccid paralysis, with frequent heart or respiratory
 CC failure (By similarity).
 CC -|- CATALYTIC ACTIVITY: Limited hydrolysis of proteins of the
 CC neuroexocytosis apparatus, synaptobrevins, SNAP25 or syntaxin. No
 CC detected action on small molecule substrates.
 CC -|- SUBUNIT: Disulfide-linked heterodimer of a light chain (L) and a
 CC heavy chain (H) (By similarity).
 CC -|- SUBCELLULAR LOCATION: Secreted protein.
 CC -|- MISCELLANEOUS: There are seven antigenically distinct forms of
 CC botulinum neurotoxin: Types A, B, C1, D, E, F, and G.
 CC -|- SIMILARITY: Belongs to the peptidase M27 family.
 CC -----
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 CC -----
 DR EMBL; X73423; CAA51824.1; -; Genomic_DNA.
 DR EMBL; X87974; CAA61234.1; -; Genomic_DNA.
 DR PIR; I40645; I40645.
 DR PDB; 1E1H; X-ray; A/C=1-249, B/D=250-415.
 DR MEROPS; M27.002; -.
 DR InterPro; IPR011591; Botulinum.
 DR InterPro; IPR008985; ConA_like_lec_gl.
 DR InterPro; IPR013320; ConA_like_subgrp.
 DR InterPro; IPR011065; Kunitz_like.
 DR InterPro; IPR006025; Pept_M_Zn_BS.
 DR InterPro; IPR000395; Peptidase_M27.
 DR InterPro; IPR013104; Toxin_rcpt_bd_C.
 DR InterPro; IPR012928; Toxin_rcpt_bd_N.
 DR InterPro; IPR012500; Toxin_trans.
 DR Pfam; PF01742; Peptidase_M27; 1.
 DR Pfam; PF07951; Toxin_R_bind_C; 1.
 DR Pfam; PF07953; Toxin_R_bind_N; 1.
 DR Pfam; PF07952; Toxin_trans; 1.
 DR PRINTS; PR00760; BONTOXILYSIN.
 DR ProDom; PD001963; Botulinum; 1.
 DR PROSITE; PS00142; ZINC_PROTEASE; FALSE_NEG.
 KW 3D-structure; Hydrolase; Membrane; Metal-binding; Metalloprotease;
 KW Neurotoxin; Protease; Toxin; Transmembrane; Zinc.
 FT INIT_MET 0 0 By similarity.
 FT CHAIN 1 447 Botulinum neurotoxin A light-chain.
 FT /FTid=PRO_0000029213.
 FT CHAIN 448 1295 Botulinum neurotoxin A heavy-chain.
 FT /FTid=PRO_0000029214.

FT	TRANSMEM	626	646	Potential.
FT	TRANSMEM	655	675	Potential.
FT	ACT_SITE	223	223	By similarity.
FT	METAL	222	222	Zinc (catalytic) (By similarity).
FT	METAL	226	226	Zinc (catalytic) (By similarity).
FT	DISULFID	429	453	Interchain (between light and heavy
FT				chains) (By similarity).
FT	DISULFID	1234	1279	By similarity.
FT	TURN	9	10	
FT	STRAND	15	22	
FT	TURN	24	25	
FT	TURN	27	28	
FT	STRAND	32	38	
FT	TURN	39	40	
FT	STRAND	41	47	
FT	STRAND	50	51	
FT	TURN	53	54	
FT	STRAND	57	57	
FT	STRAND	59	59	
FT	STRAND	62	63	
FT	STRAND	67	68	
FT	STRAND	72	72	
FT	TURN	74	77	
FT	STRAND	79	79	
FT	HELIX	80	98	
FT	TURN	99	99	
FT	STRAND	100	100	
FT	HELIX	101	112	
FT	STRAND	118	118	
FT	STRAND	121	122	
FT	TURN	123	124	
FT	STRAND	125	127	
FT	TURN	130	131	
FT	STRAND	132	137	
FT	TURN	139	140	
FT	STRAND	141	141	
FT	STRAND	143	147	
FT	STRAND	149	154	
FT	STRAND	157	158	
FT	TURN	159	160	
FT	STRAND	163	165	
FT	STRAND	167	168	
FT	TURN	171	172	
FT	TURN	174	176	
FT	STRAND	177	178	
FT	STRAND	183	186	

FT TURN	189	190
FT STRAND	191	197
FT STRAND	210	213
FT HELIX	216	231
FT TURN	232	233
FT TURN	238	239
FT STRAND	241	245
FT STRAND	253	258
FT HELIX	259	265
FT HELIX	267	272
FT STRAND	273	273
FT HELIX	275	298
FT STRAND	301	302
FT STRAND	304	307
FT HELIX	309	320
FT TURN	321	321
FT STRAND	323	324
FT TURN	326	327
FT STRAND	328	328
FT STRAND	330	331
FT HELIX	334	346
FT TURN	347	347
FT STRAND	348	348
FT HELIX	350	357
FT TURN	358	358
FT STRAND	363	365
FT STRAND	372	374
FT STRAND	378	379
FT TURN	380	382
FT STRAND	384	384
FT TURN	385	387
FT STRAND	388	388
FT TURN	389	389
FT TURN	395	396
FT STRAND	397	398
FT TURN	399	400
FT HELIX	401	403
FT STRAND	404	404
FT TURN	405	408
FT HELIX	409	411
FT STRAND	413	414
SQ SEQUENCE	1295 AA; 149280 MW; 5DA04A13D98D6372 CRC64;	

Query Match 70.6%; Score 4140; DB 1; Length 1295;
 Best Local Similarity 90.9%; Pred. No. 3.2e-196;
 Matches 790; Conservative 36; Mismatches 43; Indels 0; Gaps 0;

Qy 3
FVNKQFNYPVNGVDIAYIKIPNAGQMOPVKAFKIHNKIWVIPERDTFTNPEEG
DLNPP 62

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Db 2
FVNKQFNYPVNGVDIAYIKIPNAGQMOPVKAFKIHNKIWVIPERDTFTNPEEG
DLNPP 61

Qy 63
PEAKQVPVSYDSTYLSTDNEKDNLYLKGVTCLFERIYSTDLGRMLLTSIVRGIPF
WGGST 122

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Db 62
PEAKQVPVSYDSTYLSTDNEKDNLYLKGVTCLFERIYSTDLGRMLLTSIVRGIPF
WGGST 121

Qy 123
IDTELKVIDTNCINVIQPDGSYRSEELNLVIIGPSADIIQFECKSFGHEVLNLTRNGY
GS 182

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Db 122
IDTELKVIDTNCINVIQPDGSYRSEELNLVIIGPSADIIQFECKSFGHDVLNLTRNGY
GS 181

Qy 183
TQYIRFSPDFTFGFEESLEVDTNPLLGAAGKATDPAVTLAHELIHAGHRLYGIAIN
PNRV 242

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Db 182
TQYIRFSPDFTFGFEESLEVDTNPLLGAAGKATDPAVTLAHELIHAEHRLYGIAINP
NRV 241

Qy 243
FKVNTNAYYEMSGLEVSFEELRTFGGHDAKFIDSLQENEFRLYYYNKFKDIASLT
LNKAKS 302

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Db 242
FKVNTNAYYEMSGLEVSFEELRTFGGHDAKFIDSLQENEFRLYYYNKFKDVAST
LNKAKS 301

Qy 303
IVGTTASLQYMKNVFKKYLSEDTSGKFSVDKLFKLYKMLTEIYTEDNFVK
FFKVLN 362

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Db 302
IIGTTASLQYMKNVFKEKYLLSEDTSGKFSVDKLFKLYKMLTEIYTEDNFVNF
FKVIN 361

Qy 363
RKTYLNFDKAVFKINIVPKVNYTIYDGFNLRNTNLAANFNGQNTTEINNMNFTKL
KNFTGL 422

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Db 362
RKTYLNFDKAVFRINIVPDENYTIKDGFNKLGANLSTNFNGQNTTEINSRNFTRLK
NFTGL 421

Qy 423
FEFYKLLCVRGIHITSKTKLVPRGSNKALNDLCIKVNNWDLFFSPSEDNFTNDLNK
GEEIT 482

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Db 422
FEFYKLLCVRGIHPFKTKSLDEGYNKALNDLCIKVNNWDLFFSPSEDNFTNDLKD
VEEIT 481

Qy 483
SDTNIEAAEENISLDLIQQYYLTFNFDNEPENISIENLSSDIIGQLELMPNIERFPNGK
K 542

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Db 482
ADTNIEAAEENISLDLIQQYYLTFDFDNEPENISIENLSSDIIGQLEPMPNIERFPNG
KK 541

Qy 543
YELDKYTMFHYLRAQEFEGHKSRIALTNSVNEALLNPSRVYTFSSDYVKKVVK
ATEAAM 602

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Db 542
YELDKYTMFHYLRAQEFEGHGSRIILTNSAEEALLKPNVAYTFSSKYVKKINKA
VEAFM 601

Qy 603
FLGWVEQLVYDFTDETSEVSTTDKIADITHIIPYIGPALNIGNMLYKDDFVGALIFS
GAV 662

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Db 602
FLNWAEELVYDFTDETNEVTTMDKIADITHIIPYIGPALNIGNMLSKEFVEAIIFT
GVV 661

Qy 663
ILLEFIPEIAIPVLGTFALVSYIANKVLTVQTIDNALSKRNEKWDEVYKYIVTNWL
AKVN 722

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Db 662
AMLEFIPEYALPVFGTFAIVSYIANKVLTVQTINNALSKRNEKWDEVYKYTVTN
WLAKVN 721

Qy 723
TQIDLIRKKMKEALENQAEATKAIINYQYNQYTEEEKNNINFNIDDLSSKLNESIN
KAMI 782

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Db 722
TQIDLIREKMKKALENQAEATKAIINYQYNQYTEEEKNNINFNIDDLSSKLNESIN
SAMI 781

Qy 783
NINKFLNQCSVSYLMNSMIPYGVKRLEDASLKDALLKYIYDNRGTLIGQVDR
LKDKVN 842

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Db 782
NINKFLDQCSVSYLMNSMIPYAVKRLKDFDASVRDVLLKYIYDNRGTLVLQVDR
LKDEVN 841

Qy 843 NTLSTDIPFQLSKYVDNQRLSTFTEYIK 871

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Db 842 NTLSADIPFQLSKYVDNKKLLSTFTEYIK 870